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on

ENERGETICS AND TOPOGRAPHY OF INTERFACE PHENOMENA

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13. ABSTRACT

An entirely new foundation for the investigation of interfaces has been laid and partially consolidated via 42 scientific publications plus the support and development of 14 Ph.D. students. By detailed investigation of the five component parts of the excess free energy of an interface, it has been possible to clearly model many complex multi-parameter, multi-variable processes taking place at interfaces. Significant accomplishments relate to new approaches to stress corrosion cracking, surface creation during phase transformations and to a realistic model for crystal-liquid interfaces.

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FINAL REPORT

The Energetics, Kinetics and Topography of Interfaces

Grant [redacted]-AFOSR-68-1360

A. Original Objectives

The objective of this research was to theoretically analyze and experimentally investigate the various contributions which comprise the energy of both a stationary or moving interface between two phases plus how this energy changes with the detailed topography and chemical composition of the interface. It was further designed to reveal the important role these considerations, extended to include point and line defects, play in those processes that are surface controlled.

B. General Accomplishments

An entirely new foundation for the investigation of interfaces has been laid and partially consolidated. By detailed investigation of the five component parts of the excess free energy of an interface, it has been possible to clearly model many complex multi-parameter, multi-variable processes taking place at interfaces. This understanding will be of significant aid to many application areas: processing (phase transformations, foams, emulsions, aerosols, catalysis, coagulation); protection (coatings, paints); adhesion (joining, brazing); corrosion and degradation; unique properties (composites, films, membranes).

A very tangible result has been some 40-50 publications of which over half are already in print whereas the remainder are still in the manuscript stage and have either been submitted or will be submitted during the next three months. Another important consequence of this work has been the support and scientific development of 14 Ph.D. students (6 overlapping from the previous "Crystallogenics" grant).

C. Significant Accomplishments

(a) The development of an entirely new theoretical procedure for evaluating the cost of surface creation during phase transformations. This allows, for the first time, a procedure for assessing the stability of faceted interfaces and interface anisotropy effects during phase transformations.

(b) The development of a simple yet powerful model of how a hydrogen pump could operate during stress corrosion cracking. This is part of a novel new approach to stress corrosion which treats it theoretically as an interface instability problem and analyzes it after the manner of a phase transformation.

(c) The development of a realistic model of a liquid for treating crystal-liquid interactions whether it be for crystallization application or corrosion application. This "mobile-liquid" model is a significant advance over the standard "lattice-liquid" model in present use.

D. Professional Personnel Associated with this Grant

Professor William A. Tiller, Principal Investigator
Professor G. Marshall Pound
Dr. B. K. Jindal, Research Associate
Mr. R. Asaro, Research Assistant
Mr. L. Donaghey, " "
Mr. G. Geering, " "
Mr. R. Hiskes, " "
Mr. E. Holzmann, Research Associate
Mr. H. S. Kim, Research Assistant
Mr. G. Kotler, " "
Mr. K. Majumder, " "
Mr. D. Nason, " "
Mr. W. Oldfield, Research Associate
Mr. M.V. Rao, Research Assistant
Mr. J. Schumacher, " "
Mr. T. Takahashi, " "
Mr. L. Tarshis, " "

Thesis Titles

Interface Morphology Considerations During Solidification; L. A. Tarshis; Ph.D., January 1968.

Theoretical Investigations of Dendritic Growth; G. Kotler; Ph.D., January 1968.

Interfacial Electrical and Non-Equilibrium Phenomena Influencing Phase Transformations; B. Jindal; Ph.D., June 1968.

Nucleation Phenomena in the Liquid of Solid Transformation; T. Takahashi; Ph.D., June 1968.

The Role of Dendrites in Spherulitic Crystallization; G. Geering; Ph.D., June 1968.

Generation of Chemical Potentials by Analysis of Phase Diagrams; R. Hiskes; Ph.D., June 1968.

Eutectic-Type Phase Transformation. The Evaluation of their Solute Distribution and Stationary-State Morphologies; L. Donaghey; Ph.D., January 1969.

On Dendritic Growth; W. Oldfield; Ph.D., January 1969.

On Dendritic Growth; E. Holzmann; Ph.D., June 1969.

The Structure of Solid-Liquid Interface; D. Nason; Ph.D., January 1971.

Thermochemical Analysis of Phase Equilibrium in Alloy Systems; M. V. Rao; Ph.D., January 1972.

On Stress Corrosion Cracking; R. Asaro; Ph.D., June 1972.

On the Characteristics of the GaAs Solid-(Ga-As) Liquid Interface; H. S. Kim; Ph.D., June 1972.

On the Effect of Stress on Surface Electronic Properties of Metals; J. Schumacher; Ph.D., June 1972.

E. Publications

(a) Papers published in 1968:

1. Theoretical Analysis of Requirements for Crystal Growth from Solution, W. A. Tiller, J. of Crystal Growth 2, 69 (1968).

2. On Electrostatic Potentials at the Ice/Water Interface, B. K. Jindal and W. A. Tiller, Surface Science 9, 137 (1968).

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(c) Papers published in 1970:

29. A Critique on the Mathematical Theory of Spinodal Decomposition, W. A. Tiller, G. M. Pound and J. P. Hirth, Acta Met. 18, 225 (1970).

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(d) Papers published in 1971:

39. On the Lattice-Liquid Model for Interface Roughening, D. Nason and W. A. Tiller, J. of Crystal Growth 10, 117 (1971).

40. Equivalent Conductivity of Potassium Halides in Molten Acetamide, R. A. Wallace, J. Phys. Chem. 75, 2687 (1971).

41. Structural Transition in Strong-Acid Membranes, R. A. Wallace and B. K. Jindal, J. of Electrochem. Soc. 118, 707 (1971).

42. Further Comments on Spinodal Decomposition, W. A. Tiller, G. M. Pound and J. P. Hirth, Acta Met. 19, 475 (1971).

(e) Papers accepted for publication:

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2. On the Energetics, Kinetics & Topography of Interfaces, W. A. Tiller, "Solidification," ASM, December 1971.

3. On Surface Creation During Phase Transformations, W. A. Tiller and B. K. Jindal, Acta Met., 1972.

4. Freezing Potentials, I: Effect of Substrate on Potential During the Freezing of Aqueous Solutions at a Uniform Rate, B. K. Jindal and W. A. Tiller, J. of Colloid and Interface Science, 1972.

5. The System In-Ga: Thermodynamics and Computed Phase Equilibria, M. V. Rao and W. A. Tiller, J. of Mats. Sci., 1972.

(f) Papers submitted for publication:

1. Transient Electrical Potentials at Ice-Sodium Polystyrene Sulfonate Solution Interface, B. K. Jindal and R. A. Wallace, J. of Colloid and Interface Science.

2. On the Critical Size Dependence of Tarnish Films During the Stress Corrosion of α-Brass, R. J. Asaro, Phil. Mag.

3. Interface Morphology Development During Stress Corrosion Cracking, Part I: Via Surface Diffusion, R. J. Asaro and W. A. Tiller, Metallurgical Trans.

4. On the Enthalpy and Entropy of Fusion for Simple Liquids, D. Nason and W. A. Tiller, Acta Met.

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4. On Czochralski Growth of Yag Crystals, B. K. Jindal.

5. A Mobile Liquid Model for Interface Roughening, Part I. Single-Layer Roughening, D. Nason and W. A. Tiller.

6. A Mobile Liquid Model for Interface Roughening, Part II. Multi-Layer Roughening, D. Nason and W. A. Tiller.

7. A Mobile Liquid Model for Interface Roughening, Part III. The Crystal and Liquid Transition Zones at a Smooth Interface, D. Nason and W. A. Tiller.

8. Interfacial Adsorption in Binary Systems, D. Nason and W. A. Tiller.

9. Determination of Solute Interaction Parameters in the Systems Fe-Ni, Fe-Cr and Cr-Ni, M. V. Rao and W. A. Tiller.

10. Solute Interactions in Ternary Alloys - Analysis of the System Fe-Cr-Ni, M. V. Rao and W. A. Tiller.

11. On the Thermochemistry of Solid Nickel-Chromium Alloys, M. V. Rao and E. Flores-Magon.